Introduction to Ensemble methods

- We have looked at different machine learning models now
  - k-Nearest Neighbours
  - Classification & Regression Trees (CART)
  - Logistic Regression
  - Neural Networks
  - Support Vector Machines

- Question: Given a dataset, which ML algorithm should we pick, and how do you know which technique will perform the best?

- Unfortunately, there is no good answer to this question.
  - It is mostly a process of trial-and-error
  - Each kind of ML algorithm yields a different model/hypothesis
  - But there is no perfect model/hypothesis in practice

- So you may ask could we combine several imperfect models into a better model?

- Analogies of combining multiple models in our society
  - Elections combine voter's choices to pick a "good" candidate
  - Committees combine several experts' opinion to make better decisions

- Intuition behind combining multiple models / hypotheses
  - Individuals (or individual models) often make mistakes, but the "majority" is less likely to make mistakes
  - Individuals often have partial knowledge, but a committee can pool expertise to make better decisions

- Ensemble learning can combine an ensemble of
  - Different types of base models (e.g. Neural networks, CART and SVM)
  - Same base model trained slightly differently ✓ We are going to follow this approach

Bagging (or Bootstrap Aggregating)

- A central concept in ML is the bias-variance tradeoff
  - The more flexible a model is, the lower its bias will be
- Examples of highly flexible models that can represent complicated input-output relationships are k-Nearest Neighbours, CART, NNs, etc.
- The downside of such highly flexible models is the risk of overfitting
- Overfitted models lead to unwanted high variance in predictions
- By using bagging, we can reduce the variance of the base model without increasing its bias
- Lets take an example of regression trees with bagging

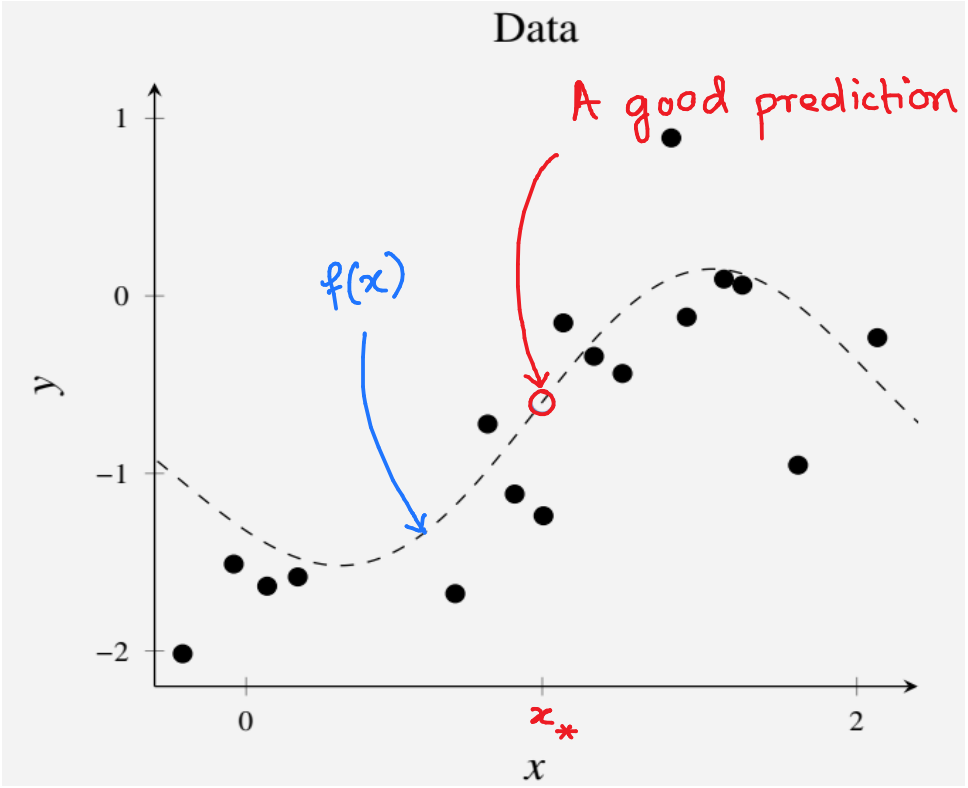
- Consider the data obtained as

$$y = f(x) + \epsilon$$

(ϵ: noise)

- We would like to train an ML model using this data, so as to be able to predict new data points well

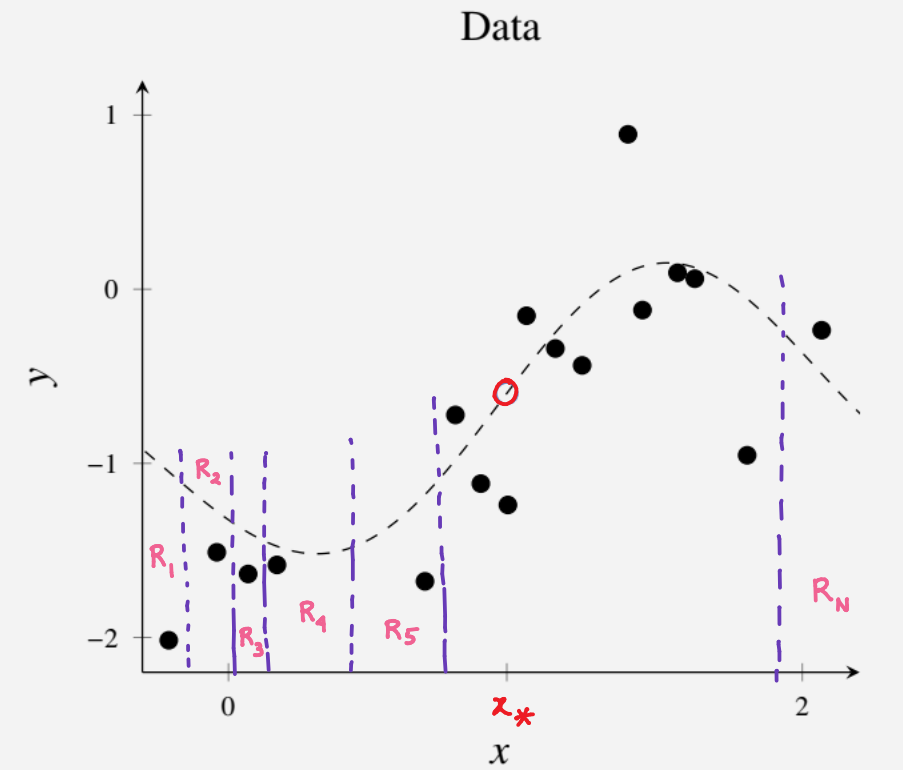
- A good prediction would mean that the trained model should predict $f(x)$ shown by the dotted line well at x_*

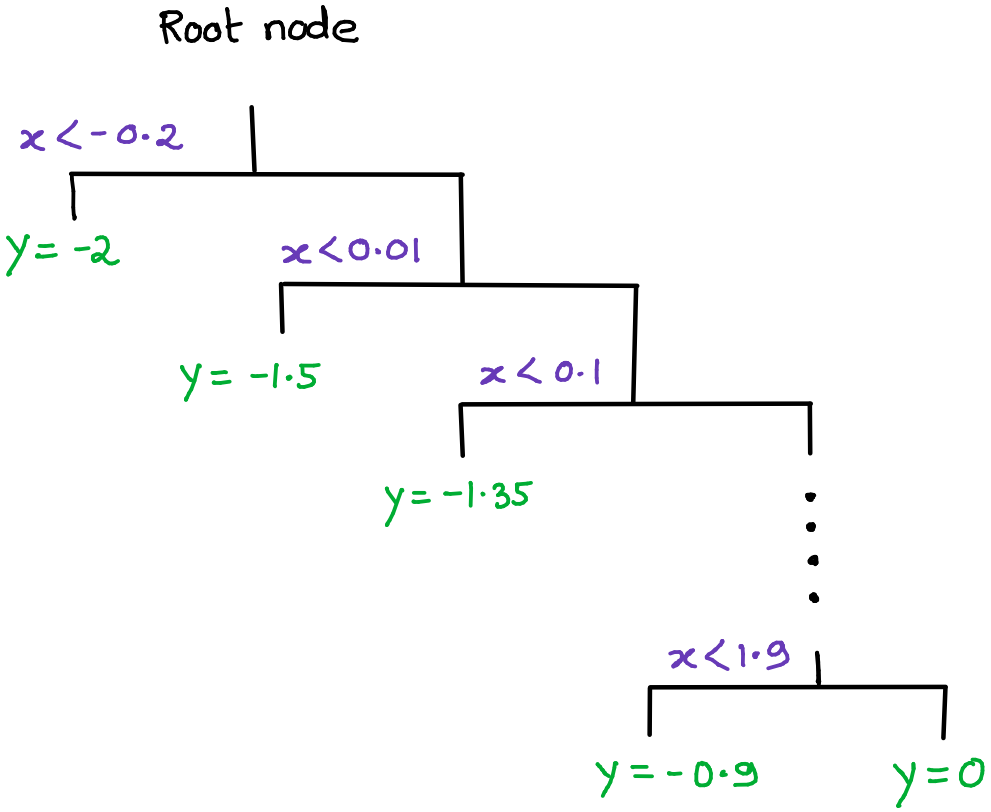


- For this problem, let us use Regression Trees as the chosen ML method, since they are non-parametric methods and are very flexible

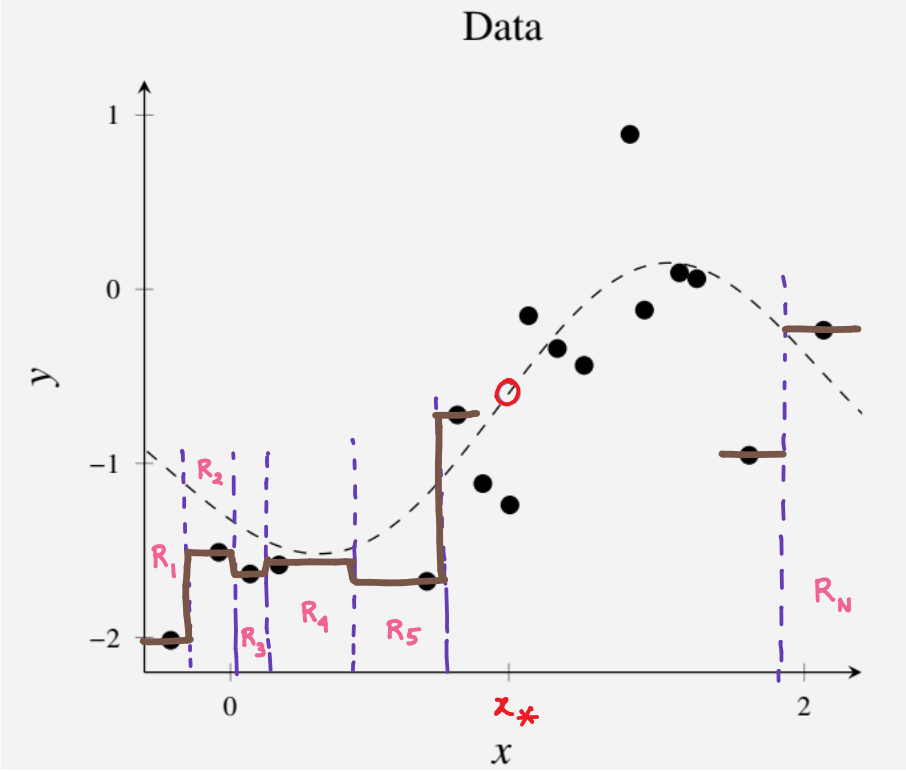
- Recall that in Classification and Regression trees, we partition the input space using box-shaped decision boundaries

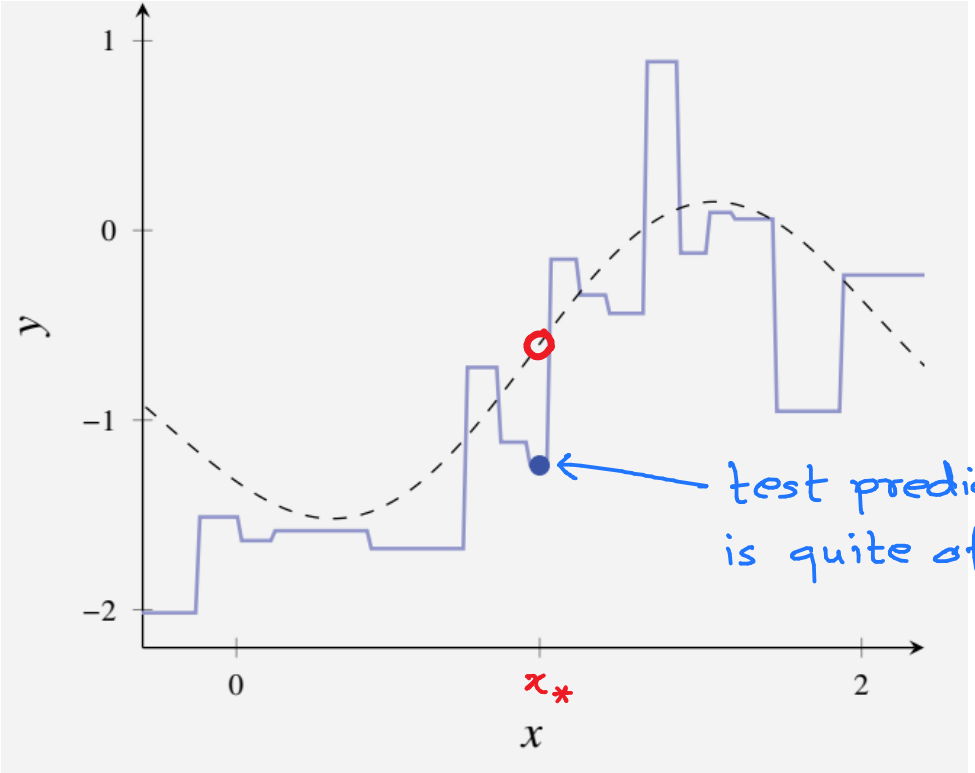
- Lets consider a Regression tree which is grown until each leaf node has only one data point





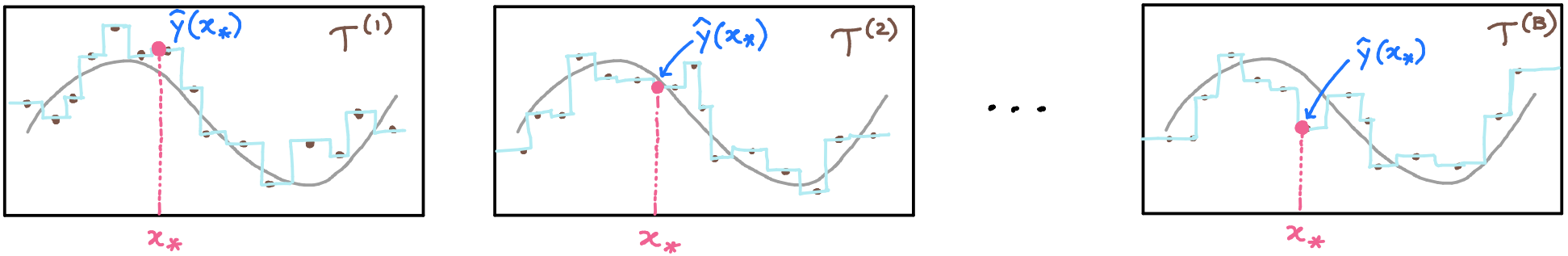
- On fitting a regression tree (with one data point in each leaf), we get an OVERFITTED Regression Tree





- Due to overfitting, the resulting regression tree is a low-bias-high-variance model
  - high variance means the trained model is very sensitive to the training data; if the training data changes, the predictions change a lot

- Because of the noise in training data, we can think of the prediction $\hat{y}(x_*)$ from the trained model as a random variable
  - It means that if we had multiple datasets and we trained different RTs on them, each of their predictions $\hat{y}(x_*)$ would be different



- So if we assumed that we had access to B independent datasets $T^{(1)}, T^{(2)}, \ldots, T^{(B)}$, then we could train a separate tree for each dataset and obtain separate predictions $\hat{y}_b(\underline{x}_*)$, $b = 1, 2, \ldots, B$, then:
  - Each $y_b(\underline{x}_*)$ would have low bias and high variance
  - By averaging $\hat{y}(\underline{x}_*) = \frac{1}{B} \sum_{b=1}^{B} \hat{y}_b(\underline{x}_*)$, the bias is kept small, but the variance is reduced by a factor of B! (HW3)

Probability detour – Variance reduction by averaging

Let $z_1, z_2, \ldots, z_B$ be a collection of identically distributed but possibly dependent random variables, with

$$\left.\begin{aligned} \text{Mean}: \quad & \mathbb{E}[z_b] = \mu \\ \text{Variance}: \quad & \text{Var}(z_b) = \sigma^2 \end{aligned}\right\} \quad \text{for } b = 1, 2, \ldots, B$$

$$\text{Correlation}: \quad \text{Corr}(z_i, z_j) = \rho \qquad i \neq j, \quad i, j = 1, 2, \ldots, B$$

Then one can show that the mean and variance of the average $\frac{1}{B}\sum_{b=1}^{B} z_b$ are: (Assume $0 < \rho < 1$)

$$\mathbb{E}\left[\frac{1}{B}\sum_{b=1}^{B} z_b\right] = \mu, \qquad \text{Var}\left[\frac{1}{B}\sum_{b=1}^{B} z_b\right] = \underbrace{\frac{1-\rho}{B}}_{\text{small for large } B}\sigma^2 + \rho\sigma^2$$

- Problem: We only have access to one training dataset
- Solution: Bootstrap the data!
- Bootstrap is a method of artificially creating multiple datasets (of size N) out of one dataset (also of size N)
  - Sample N times with replacement from the original training data $T = \{ \underline{x}_i , y_i \}_{i=1}^{N}$
  - Repeat B times to generate B "bootstrapped" training datasets $\tilde{T}^{(1)}, \tilde{T}^{(2)}, \ldots, \tilde{T}^{(B)}$
- BAGGING
  - For each bootstrapped dataset $\tilde{T}^{(b)}$, we train a tree (base model)

    Averaging them,

$$\hat{y}_{bag} = \frac{1}{B} \sum_{b=1}^{B} \tilde{y}^{b}(\underline{x})$$

Bagging example with regression trees as basemodel

Assume that we have a training set

$$\mathcal{T} = \left\{ (\underline{x}_1, y_1), (\underline{x}_2, y_2), (\underline{x}_3, y_3), \dots, (\underline{x}_N, y_N) \right\}$$

- We generate, say, $B = 9$ datasets by bootstrapping:

$$\tilde{\mathcal{T}}^{(1)} = \left\{ (\underline{x}_1, y_1), (\underline{x}_2, y_2), (\underline{x}_3, y_3), \dots, (\underline{x}_3, y_3) \right\}$$

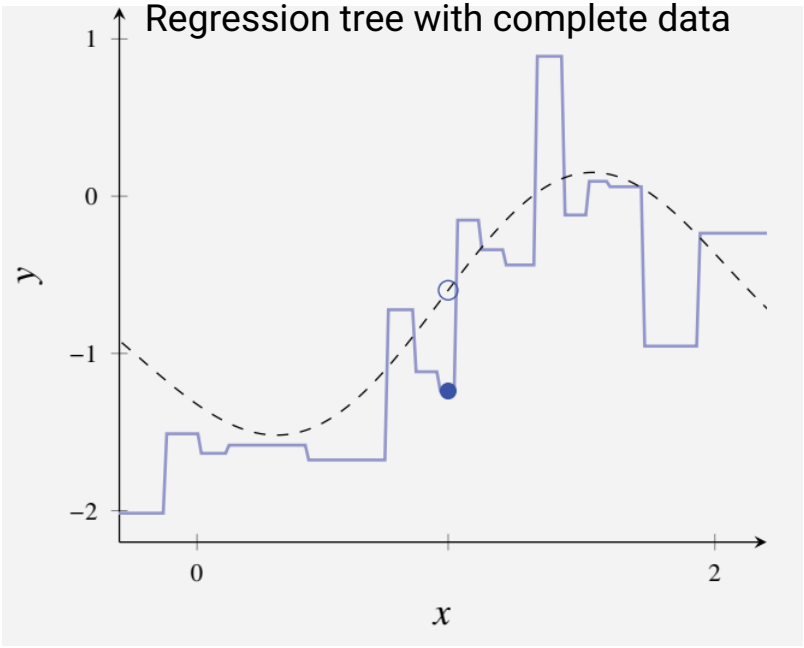
$$\tilde{\mathcal{T}}^{(2)} = \left\{ (\underline{x}_1, y_1), (\underline{x}_N, y_N), (\underline{x}_N, y_N), \dots, (\underline{x}_N, y_N) \right\}$$

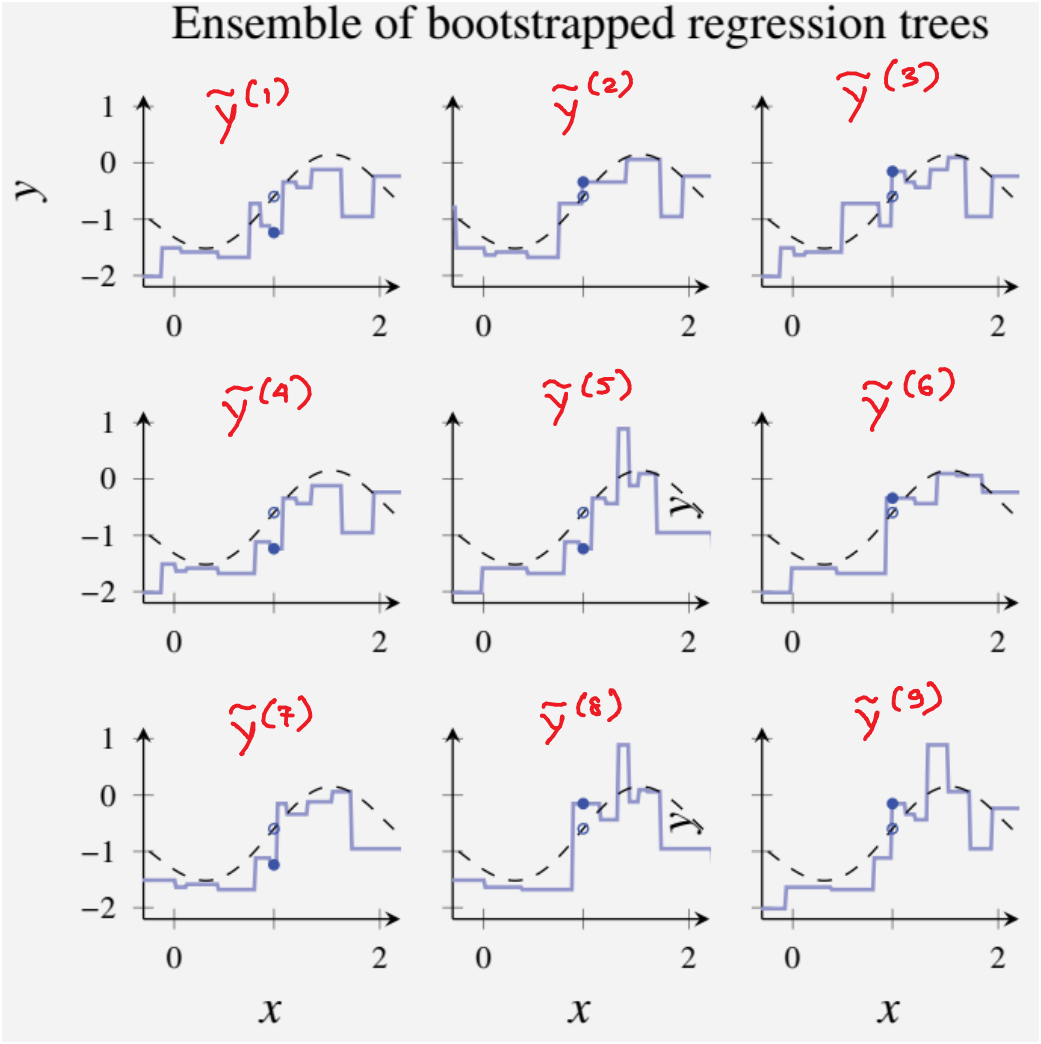
$$\vdots \qquad\qquad \vdots$$

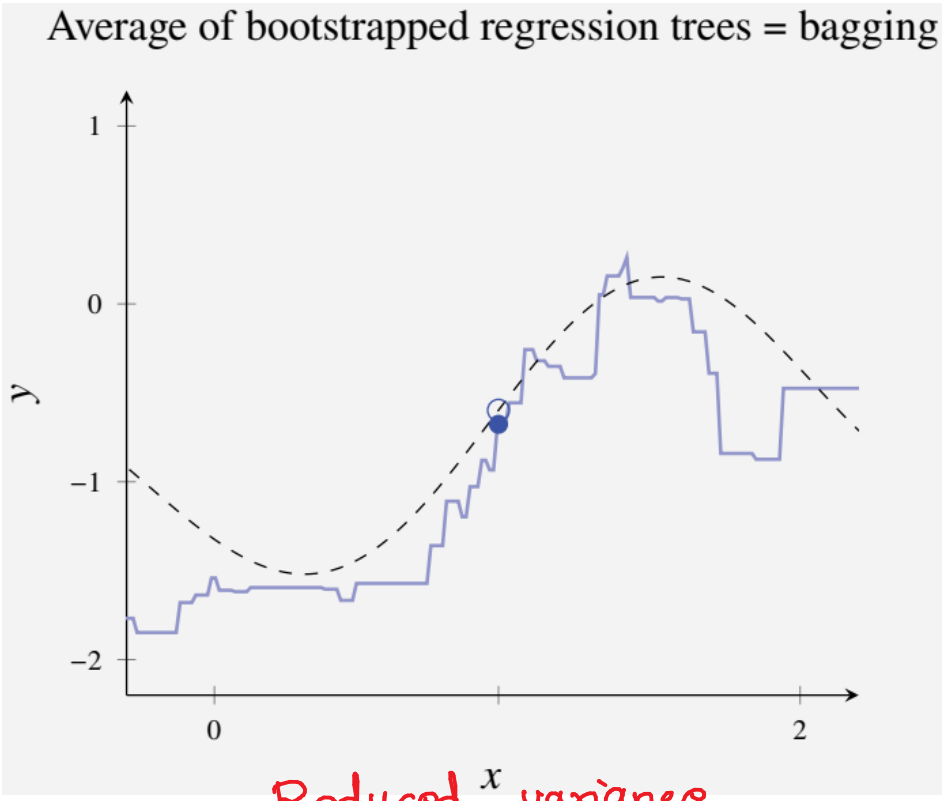
$$\tilde{\mathcal{T}}^{(9)} = \left\{ (\underline{x}_1, y_1), (\underline{x}_1, y_1), (\underline{x}_2, y_2), \dots, (\underline{x}_3, y_3) \right\}$$

- We compute $B = 9$ (deep) regression trees $\tilde{y}^{(1)}(\underline{x}), \tilde{y}^{(2)}(\underline{x}), \dots, \tilde{y}^{(9)}(\underline{x})$ one for each dataset $\tilde{\mathcal{T}}^{(1)}, \tilde{\mathcal{T}}^{(2)}, \dots, \tilde{\mathcal{T}}^{(9)}$, and average $\hat{y}_{bag} = \frac{1}{9} \sum_{b=1}^{9} \tilde{y}^{(b)}(\underline{x})$

Bagging example with regression trees







Bagging algorithm

- **Training :** Learn all base models

  Data : Training dataset $\mathcal{T} = \{ \underline{x}_i , y_i \}_{i=1}^{N}$

  Result : 'B' base models

  for $b = 1, \ldots, B$ do

  - Generate a bootstrap dataset $\tilde{\mathcal{T}}^{(b)}$ of the same size as $\mathcal{T}$
  - Learn a base model from $\tilde{\mathcal{T}}^{(b)}$

  end

  Obtain $\hat{y}_{bag}(\underline{x})$ by averaging : $\hat{y}_{bag}(\underline{x}) = \frac{1}{B} \sum_{i=1}^{B} \tilde{y}^{(b)}(\underline{x})$

The choice of 'B' is mainly guided by computational constraints

- **Prediction with the base models**

  Data : 'B' base models and test input $\underline{x}_*$

  Result : A prediction $\hat{y}_{bag}(\underline{x}_*)$

Use same formula

Random Forests

- Bagging can greatly improve the performance of CART
  - Averaging over ensemble prediction, in case of regression trees
  - Majority vote over ensemble prediction, for classification trees

- However, the 'B' bootstrapped dataset are correlated!

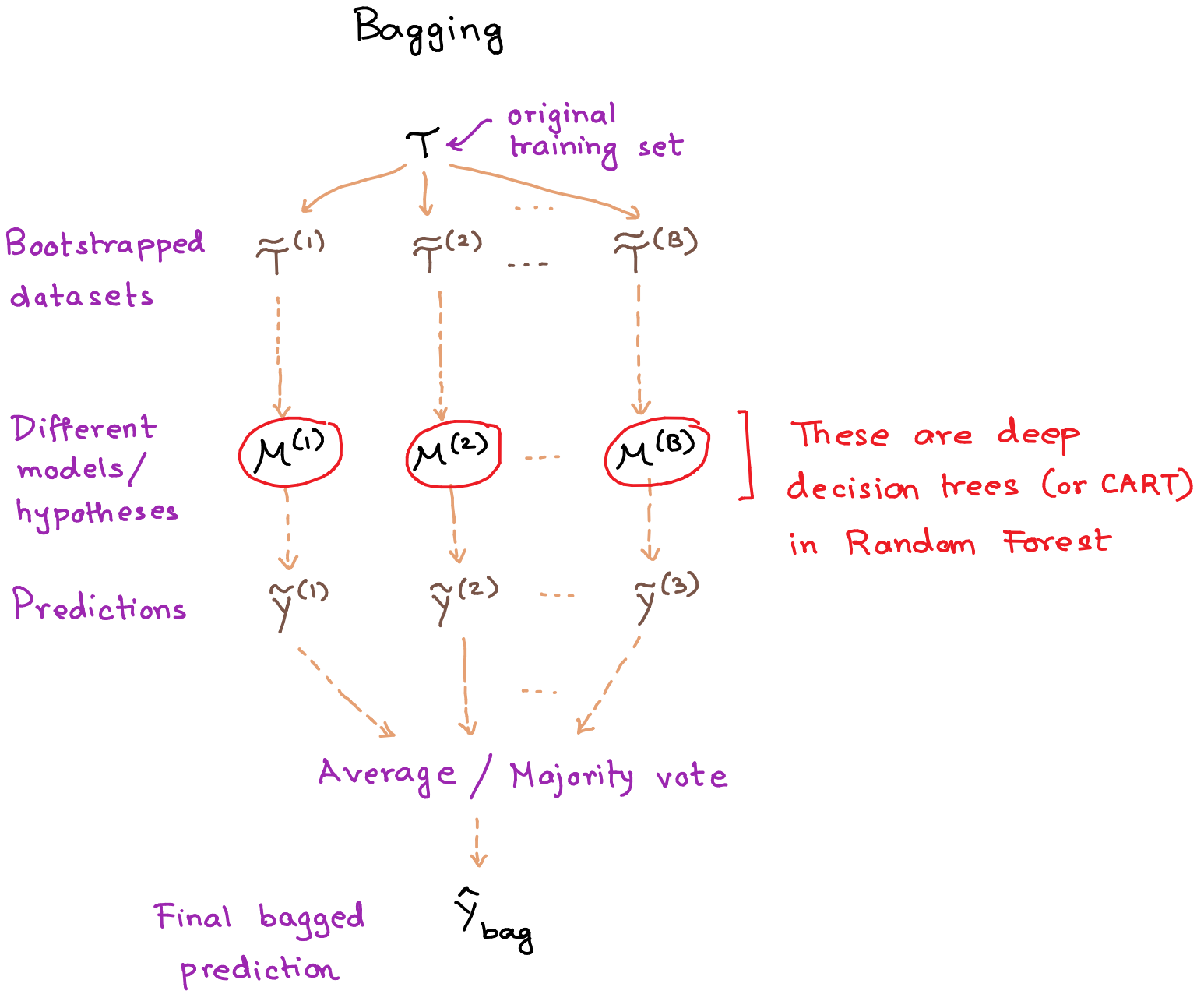
  Therefore, the variance reduction due to averaging is diminished

Recall $$\text{Var}\left[\frac{1}{B}\sum_{b=1}^{B} z_b\right] = \frac{1-\rho}{B}\sigma^2 + \rho\sigma^2$$

- No variance reduction when $\rho = 1$
- Highest variance reduction when $\rho = 0$

- Idea of Random Forest: De-correlate the 'B' trees by injecting additional randomness when constructing each tree

Random Forest = Bagging + Decision Trees with random feature subset selection



Random Feature Subsets

- While growing a decision tree, one selects the best input feature x_j from all 'p' input variables $x_1, x_2, \cdots, x_p$ for splitting a node

- In random forest, we pick a random subset consisting of $q \leq p$ features and only consider these 'q' input features for possible splits

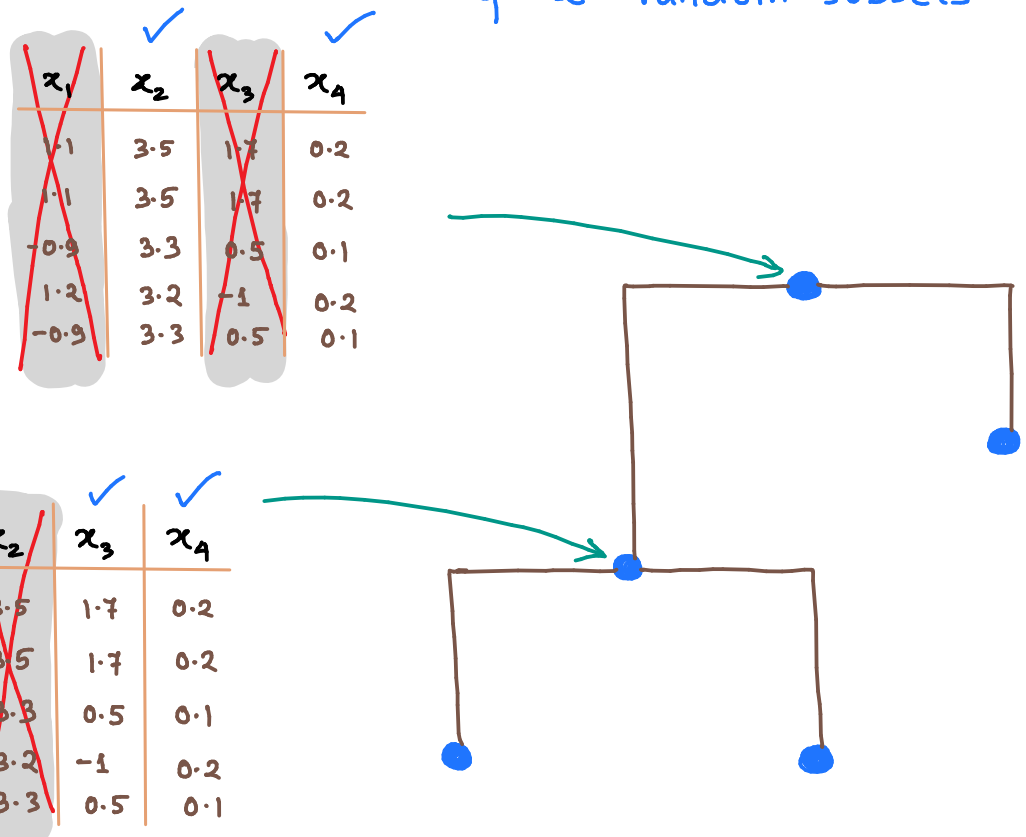
Example

A bootstrapped dataset

x_1	x_2	x_3	x_4
1·1	3·5	1·7	0·2
1·1	3·5	1·7	0·2
-0·9	3·3	0·5	0·1
1·2	3·2	-1	0·2
-0·9	3·3	0·5	0·1

p = 4 (# of inputs)

q = 2 random subsets



Random forest algorithm

Inputs: $T = \{ \underline{x}_i , y_i \}_{i=1}^{N}$; $\underline{x} \in \mathbb{R}^p$

for $b = 1$ to B, do (can run in parallel)

(a) Draw a bootstrap dataset $\tilde{T}^{(b)}$ of size N from T

(b) Grow a regression (or classification) tree by repeating the steps below, until a minimum node size is reached:

- Select a random subset consisting of $q \leq p$ inputs
- Find the best splitting variable x_j among the 'q' selected inputs
- Split the node into two children with $\{ x_j \leq s \}$ and $\{ x_j > s \}$

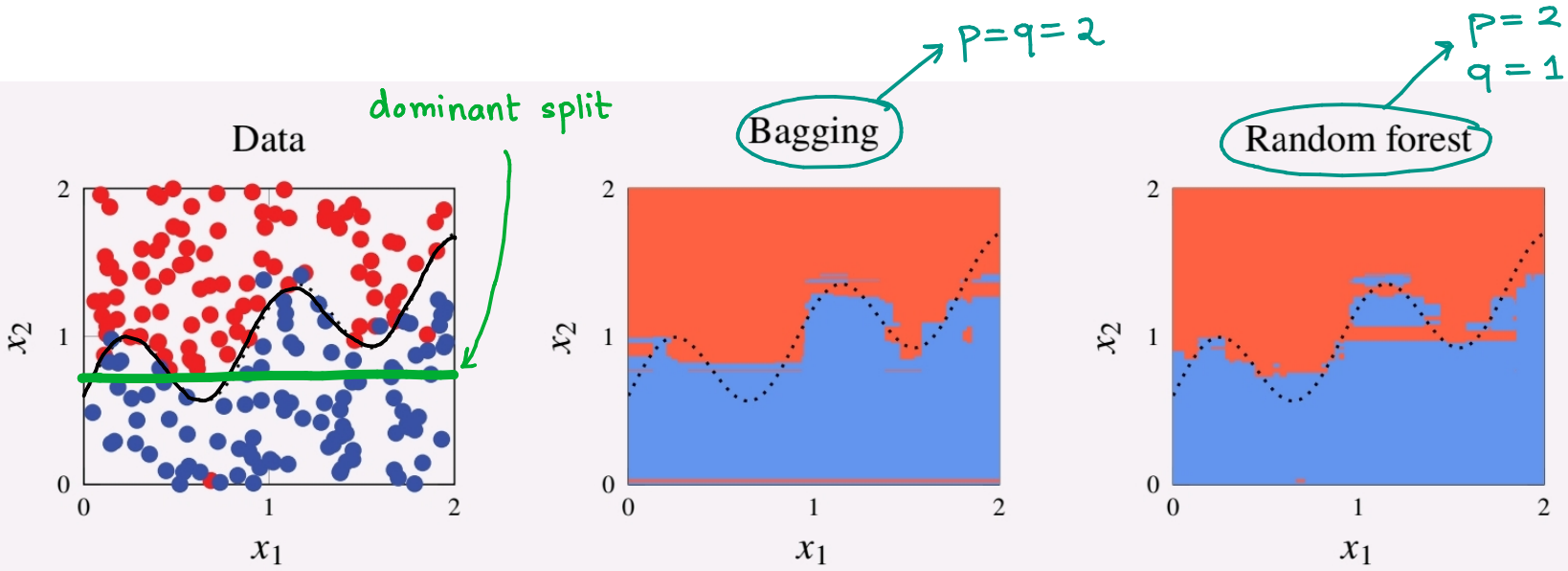
Thumb rule
$q = \sqrt{p}$ (for CT)
$q \approx p/3$ (for RT)

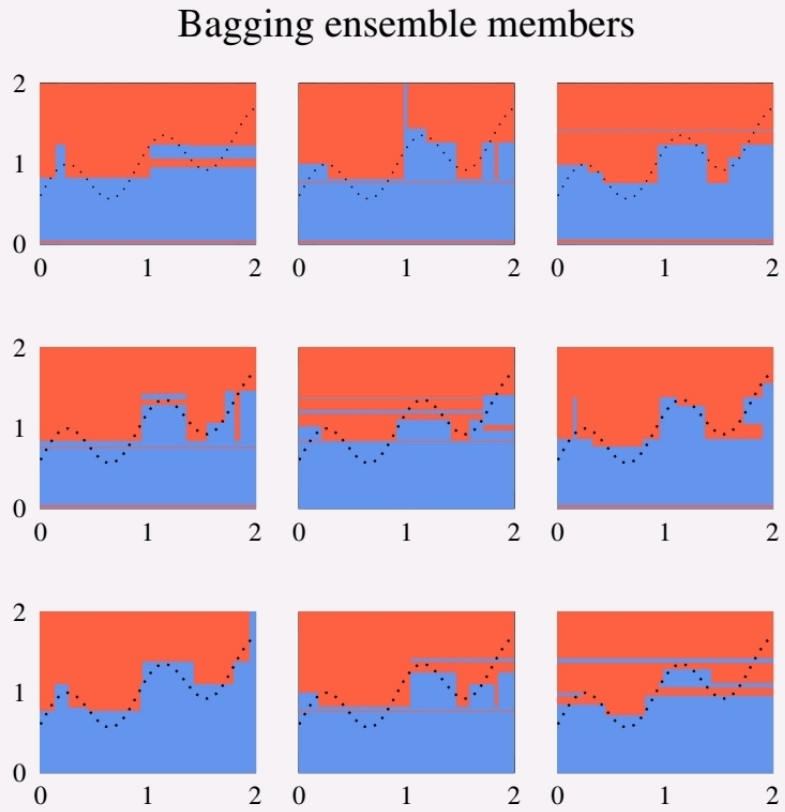
Final model is the average of the 'B' ensemble members

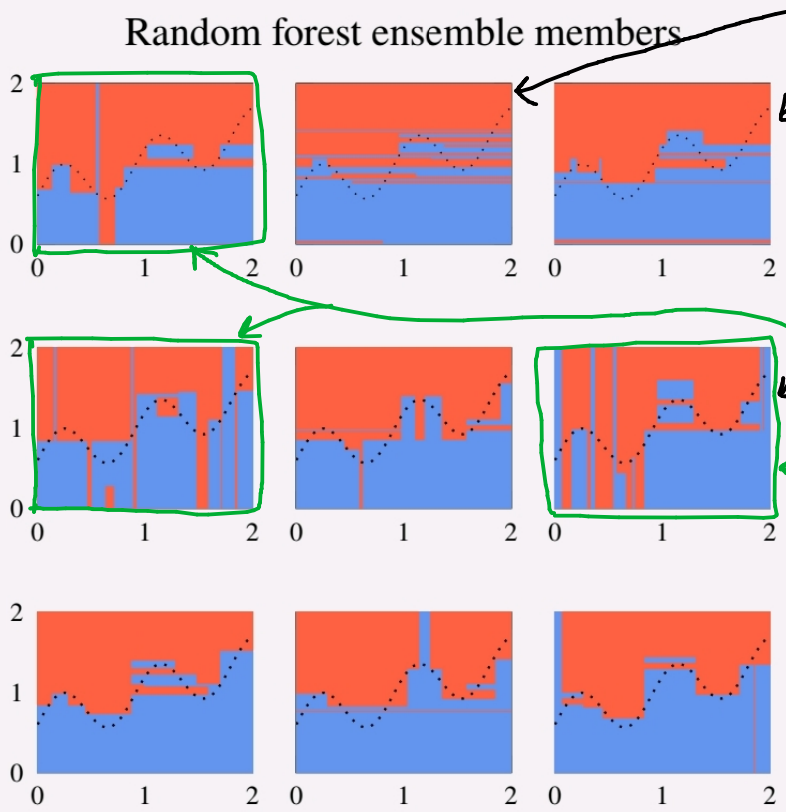
$$\hat{y}_{rf} = \frac{1}{B} \sum_{b=1}^{B} \tilde{y}^{(b)}$$

Example of binary classification

B = 9 ensemble members

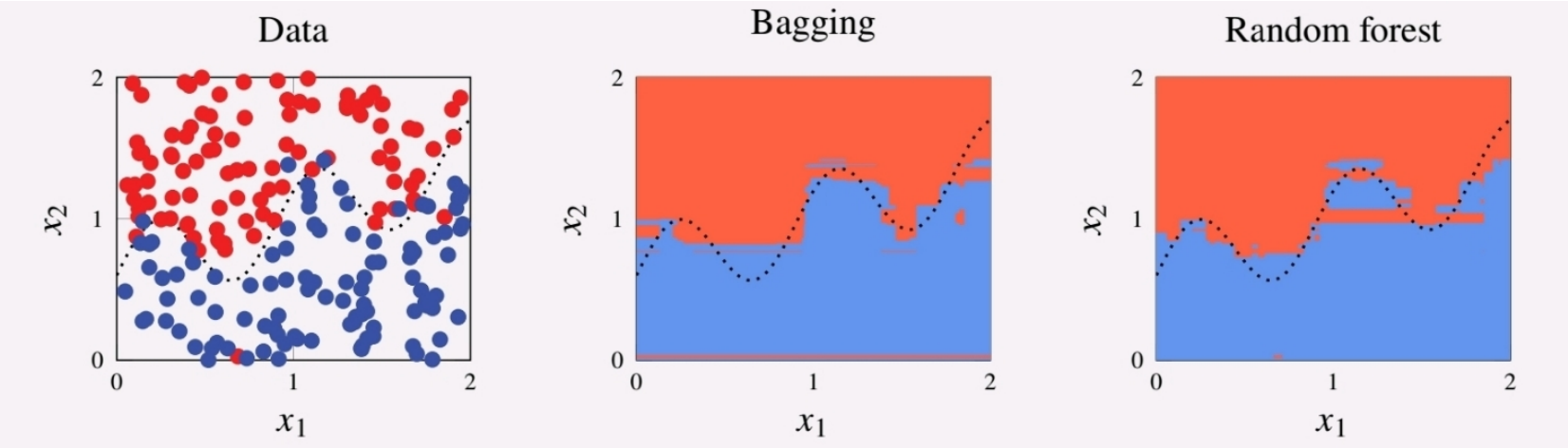




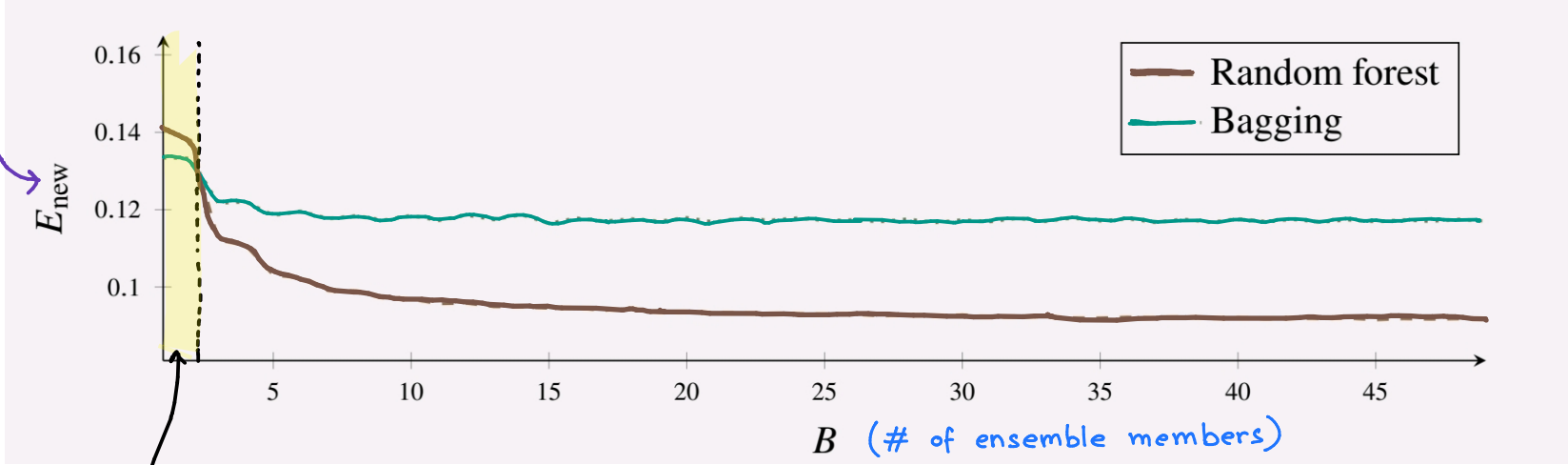


Random Forest Ensemble members have more individual variation than bagging

dominant splits along x_1



Expected New Data Error



For very small B, bagging performs better than random forests

However, as the number of ensemble member increases, test error decreases more for random forests

- For identically distributed random variables $\{z_b\}_{b=1}^{B}$

$$\text{Var}\left[\frac{1}{B}\sum_{b=1}^{B} z_b\right] = \frac{1-\rho}{B}\sigma^2 + \rho\sigma^2$$

- The random input selection used in random forests:
  - increases the bias, but often very slowly ↓
  - adds to the variance (σ^2) of each tree ↓
  - reduces the correlation (ρ) between member trees ↑↑↑

- The reduction in correlation typically has a dominant effect
  ⇒ leads to an overall reduction in error

- Bagging is a general technique → can be used with any base model

Random forests consider base models as classification or regression trees